

# **TOUGHREACT Training Course**

October 3-5, 2018 Energy Geosciences Division  
Lawrence Berkeley National Laboratory  
Berkeley, CA 94720

## **Instructors**

**Eric Sonnenthal and Nicolas Spycher**

This course will provide a hands-on introduction to the latest shared-memory parallel release of TOUGHREACT (V3.3-OMP). Sample problems include simple reactive transport in batch and flow-through systems, equilibrium and kinetic reactions, hydrothermal experiments, followed by more complex problems on geological sequestration of CO<sub>2</sub> and subsurface nuclear waste storage. These problems serve as prototypes for creating input files for new applications. The course will also include discussions of the underlying physical and chemical processes, as well as the mathematical and numerical approaches used.

# AGENDA

**Wednesday, October 3, 2018**

## **Afternoon Session**

*13:00 Introduction*

- Course objectives and outline
- TOUGHREACT V3.3-OMP installation on participant laptops

*13:15 TOUGHREACT basics*

- Overview of TOUGHREACT V3.3-OMP
- Multicomponent geochemical computations

*14:30 Problem No. 1 – Introduction to Setup of a Simple Reactive Transport Problem*

- Discussion of flow input and output files
- Discussion of chemical input and output files
- Discussion of thermodynamic data file
- Simple aqueous transport with NaCl solution

*17:00 Adjourn*

*18:30 Dinner (to be announced)*

## Thursday, October 4, 2018

- 9:00 ***Problem No. 1 - continued***
- Aqueous transport with calcite, gypsum and dolomite: Batch and flow-through
  - Different mineral zones
  - Problem variations
- 12:00 ***Lunch***
- 13:00 ***Problem No. 2 – 1-D Plug-flow reactor experiment***
- Calculation of various input data, setup of input files
  - Time discretization (Courant limitation)
  - Mesh generation (1D Cartesian)
  - Simulations with one (quartz) and more minerals (volcanic tuff)
- 17:00 ***Adjourn***

## Friday, October 5, 2018

- 9:00 ***Problem No. 3 – 1-D radial CO<sub>2</sub> injection problem (Sample Problem 5 in manual)***
- Baseline simulation
  - Flow-only simulation (no reaction)
  - Simulations with/without CO<sub>2</sub> reaction feedback on flow
  - Restart option
  - *2D X-Z mesh* problem definition
  - Setup of the chemical input files
  - Local equilibrium versus kinetics
  - Linear versus radial mesh
  - Connecting chemical zones to grid blocks
  - Preparation of initial water composition
  - Problem variations
- 12:00 ***Lunch***
- 13:00 ***Problem No. 4 – Geologic disposal of nuclear waste***
- Problem conceptualization
  - Setup of the chemical input files
  - Local equilibrium versus kinetics
  - Problem variations
- 16:30 ***Concluding Remarks and Open Discussion***
- 17:00 ***Adjourn***